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Abstract

The rise of bubbles in viscous liquids is not only a very common process in many industrial applications, but also an important fundamental problem in fluid physics. An improved numerical algorithm based on the front tracking method, originally proposed by Tryggvason and his coworkers, has been validated against experiments over a wide range of intermediate Reynolds and Bond numbers using an axisymmetric model (Hua and Lou, *J. Comput. Phys.* **222**:769-795, 2007). In the current paper, this numerical algorithm is further extended to simulate 3D bubbles rising in viscous liquids with high Reynolds and Bond numbers and large density and viscosity ratios at the physical order of the typical multi-fluid system of air bubbles in water. To facilitate the simulation, mesh adaptation is implemented for both the front mesh and the background mesh, and the governing Navier-Stokes equations for incompressible, Newtonian flow are solved in a moving reference frame attached to the rising bubble. Specifically, the flow equations are solved using a finite volume scheme based on the Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) algorithm, and it appears to be robust even in the range of high Reynolds numbers and high density/viscosity ratios. The 3D bubble surface is tracked explicitly using an adaptive, unstructured triangular mesh. The model is integrated with the software package PARAMESH, a block-based adaptive mesh refinement (AMR) tool developed for parallel computing. PARAMESH allows background mesh adaptation as well as the solution of the governing equations in parallel on a supercomputer. The interpolations between the front mesh and the background mesh are done with Peskin's distribution function. The current model has also been applied to

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simulate a number of cases of 3D gas bubbles rising in viscous liquids, e.g. air bubbles rising in water. The simulation results are compared with experimental observations both in aspect of terminal bubble shapes and terminal bubble velocities. In addition, we applied this model to simulate the interaction between two bubbles rising in a liquid. The simulation results provide us with more physical insights into the complex bubble rising behavior in viscous liquids.

Keywords*:* Computational fluid dynamics; Incompressible flow; Multiphase flow; Bubble rising; SIMPLE algorithm; Front tracking method; Adaptive mesh refinement; Moving reference frame

1. Introduction

Multiphase flows are numerous in both everyday life and engineering practice [34]. Typical examples in nature include raindrops in air and gas bubbles in water, whereas chemical reactions, combustion and petroleum refining are examples of multiphase flows in industry. One very basic example of such flow is the rise of a single gas bubble in an otherwise quiescent viscous liquid. The understanding of the flow dynamics of this system is of great importance in engineering applications and to the fundamental understanding of multiphase flow physics. Rising bubbles have long been studied theoretically [8, 25], experimentally [1] as well as computationally through numerical modeling [36]. While all these efforts have provided us with valuable insights into the dynamics of bubbles rising in viscous liquids, there are still many questions that remain unanswered due to the involvement of complex physics. The behavior of a bubble rising in a viscous liquid is not only affected by the physical properties such as density and viscosity of both phases [6], but also by the surface tension on the interface between the two phases and by the bubble shape evolution [27, 2]. The difficulties in describing and modeling the complex behavior of a rising bubble are to a large extent due to the strong nonlinear coupling of factors such as buoyancy, surface tension, bubble/liquid momentum inertia, viscosity, bubble shape evolution and rise history of the bubble. In addition, the physics of the behavior of bubbles is of a three-dimensional nature. Hence, most of the past theoretical works were done with a lot of assumptions, and the results are only valid for certain flow regimes [25, 43]. The experimental works were limited by the available technologies to monitor, probe and sense the moving bubbles without interfering with their physics [1, 38, 44].

With the rapid advance of computing power and the development of robust numerical methods, first principle based numerical simulations promise great potential in extending our knowledge of the fundamental system of a single bubble rising in a viscous liquid. However, there are still great challenges and difficulties in simulating such a system accurately. This may be attributed to the following facts: (i) the sharp interface between the gas bubble and the surrounding liquid should be tracked accurately without introducing excessive numerical smearing; (ii) the surface tension gives rise to a singular source term in the governing equations, leading to a sharp pressure jump across the

interface; (iii) the discontinuity of the density and viscosity across the fluid interface may lead to numerical instability, especially when the jumps in these properties are high. For example, the density ratio of liquid to gas could be as high as 1000; (iv) the geometric complexity caused by bubble deformation and possible topological change is the main difficulty in handling the geometry of interface; a large bubble may break up into several small ones, and a bubble may also merge with other bubbles; (v) the complex physics on the interface, e.g. the effects of surfactants, film boiling and phase change (heat and mass transfer) and chemical reactions. Fortunately, various methods for multiphase flow have been developed to address these difficulties, and each method typically has its own characteristic strengths and weaknesses. Comprehensive reviews of numerical methods for multiphase/interfacial flow simulation have been given by Scardovelli and Zaleski [37] and Annaland et al. [41]. Most of the current numerical techniques applied in the simulation of multiphase/interfacial flows have been developed with focus on the following two aspects: (i) capturing/tracking the sharp interface, e.g. interface capturing, grid fitting, front tracking or hybrid methods; and (ii) stabilizing the flow solver to handle discontinuous fluid properties and highly singular interfacial source terms, e.g. the projection-correction method [41] and the SIMPLE algorithm [6, 17].

The volume of fluid [14, 4], level-set [28, 42, 29] and phase-field [19] approaches fall into the first category of front capturing methods. In these methods the interface is captured using various volume functions defined on the grid used to solve the “one-fluid” formulation of the governing equations for multiphase flow. Since interface capturing uses the same grid as the flow solver, it is relatively easy to implement. However, the accuracy of this approach is limited by the numerical diffusion from the solution of the convection equation of the volume function. Various schemes have been developed to advect, reconstruct / reinitialize the volume function to improve the accuracy in calculating the interface position. One example is the high-order shock-capturing scheme used to treat the convective terms in the governing equations [18]. Although the explicit reconstruction of the interface is circumvented, the implementation of such high-order schemes is quite sophisticated, and they do not work well for the sharp discontinuities encountered in multiphase/interfacial flows. In addition, a relatively fine grid is needed in the vicinity of the interface to obtain good resolution.

The second category of approaches tries to track the moving interface by fitting the background grid points to the interface. The fitting is achieved through re-meshing techniques such as deforming, moving, and adapting the background grid points. This method is also well-known as “boundary-fitting approach”, and the “boundary” here refers to the interface between the fluids. The grid-fitting approach is capable of capturing the interface position accurately. Early development on this approach was done by Ryskin and Leal [36]. Curvilinear grids were used to follow the motion of a rising bubble in liquid. This method is suitable for relatively simple geometries undergoing small deformations, and applications to complex, fully three-dimensional problems with unsteady deforming phase boundaries are very rare. This is mainly due to difficulties in maintaining the proper volume mesh quality and in handling complex interface geometry such as topological change. In spite of these difficulties, recent work by Hu et al. [16] showed some very impressive results on 3D simulations of moving spherical particles in liquid.

The third category is the front tracking method. This approach solves the flow field on a fixed grid and tracks the interface position in a Lagrangian manner by a set of interface markers. These interface markers can be free particles without connection, or they can be logically connected elements, possibly containing accurate geometric information about the interface such as area, volume, curvature, deformation, etc. A front tracking technique was proposed by pioneer researchers Glimm and his coworkers [11, 12, 13]. They represent the front interface using a set of moving markers and solve the flow field on a separate background grid. The background grid is modified only near the front to make background grid points coincide with the front markers of the interface. In this case, some irregular grids are reconstructed and special finite difference stencils are created for the flow solver, increasing the complexity of the method and making it more difficult to implement. Independently, another front tracking technique was developed by Peskin and collaborators [31, 10]. In their method, the interface is represented by a connected set of particles which carry forces, either imposed externally or adjusted to achieve a specific velocity at the interface. A fixed background grid is kept unchanged even near the front interface, and the interface forces are distributed onto the background to solve the “one-fluid” formulation of the fluid flow.

A number of combinations and improvements of these basic approaches have been proposed to enhance the capabilities in dealing with the sharp, moving interface, where complex physical phenomena and processes could occur. One of the most promising approaches is arguably the front tracking method proposed by Tryggvason and his collaborators [46, 45]. Actually, this method may be viewed as a hybrid of the front capturing and the front-tracking techniques: a fixed background grid is used to solve the fluid flow, while a separate interface mesh is used to track the interface position explicitly. The tracked interface carries any jumps in the fluid properties, such as density and viscosity, and any interfacial forces, such as surface tension. Fluid properties are then distributed onto the fixed background grid according to the position of the interface. The surface tension can be calculated according to the geometry of the interface and is also distributed onto the background grid in the vicinity of the interface.

Besides the numerical techniques employed to capture/track the moving interface, it is also very important to develop a stable numerical method to solve the governing equations of the flow field. Some investigators have considered simplified models such as Stokes flow [33], where inertia is completely ignored, and inviscid potential flow [15], where viscous effects are ignored in. In both cases, the motion of deformable boundaries can be simulated with boundary integral techniques. However, when considering the transient Navier-Stokes equations for incompressible, Newtonian fluid flow, the so-called "one-fluid" formulation for multiphase flow has proved most successful [4, 42, 46]. Popular modern methods that use the "one-fluid" formulation include the projection-correction method [45, 41] and the SIMPLE algorithm [6, 17]. Various multiphase/interfacial flow problems have been successfully simulated by the front tracking method [45] with a projection-correction flow solver. It appears that previously reported results have been limited to flows with low to intermediate Reynolds numbers (<100) and small density ratios (<100) [5]. It is thus natural to re-examine the approach and to make it more robust and applicable to wider flow regimes. Some revised versions of the project-correction method have been proposed to improve its capability in handling situations with large density and viscosity ratios [41]. Recently, Hua and Lou [17] tested a SIMPLE-based algorithm to solve the incompressible Navier-Stokes equations. The simulation results indicated that the newly proposed method could robustly solve the

Navier-Stokes equations with large density ratios up to 1000 and large viscosity ratios up to 500.

Hua and Lou [17] presented extensive simulations and model validation on a single bubble rising in a quiescent liquid. The comprehensive simulations show good results in wide flow regimes with high density and viscosity ratios, and the algorithm is as such promising in the direct numerical simulation of multiphase flow. Unfortunately, the previous validation studies were limited to the 2D axisymmetric model where fluid flows and bubble shapes are axisymmetric. Hence, it would be interesting to investigate the robustness of the proposed numerical approach for multiphase flow in flow regimes of higher Reynolds and Bond numbers where the bubble may not be axisymmetric anymore. Therefore, a fully three-dimensional modeling approach is proposed in this paper. In addition, other features such as mesh adaptation, moving reference frame and parallel programming are introduced to enhance the model capability in simulating the rise of a 3D bubble in a viscous liquid.

The numerical algorithm proposed by Tryggvason and co-workers [46, 45], and extended further by Hua and Lou [17], is adopted in this paper. The handling of the moving interface in this method may be characterized as a hybrid of interface tracking and capturing. The governing Navier-Stokes equations are solved on a fixed Cartesian grid with an adaptive block structure, while the interface is represented by a set of explicitly tracked front markers. These markers form an adaptive triangular surface mesh that is advected with a velocity interpolated from the surrounding fluid. An illustration of such a mesh system is shown in Figure 1. A single set of the governing equations are solved in the entire computational domain by treating the two fluids as one single fluid with variable fluid properties across the interface – often referred to as the “one-field” or “one-fluid” approach. The interface is assumed to have a given finite thickness (normally about two to four times the background grid size) so that jumps in the fluid properties across the surface can be reconstructed smoothly by solving a Poisson equation.

A parallel adaptive mesh refinement (AMR) tool, PARAMESH [24], is integrated with the modified SIMPLE flow solver, and the governing equations are solved in a non-inertial moving reference frame attached to the rising bubble. The AMR feature allows a relatively high-resolution mesh in the vicinity of the bubble surface. The non-inertial

moving reference frame technique translates the computational domain with the rising bubble, allowing the computational domain to be relatively small and always centered around the bubble. The latter feature is particularly useful for studying the path instability of a rising bubble or the interaction of multiple bubbles, which may need very long simulation periods. For example, it is observed in experiments that the paths of millimeter-sized, rising air bubbles in water normally stabilize after a rise distance of 50-100 times the initial bubble diameter. If a stationary frame was to be applied to simulate this situation, the computational domain would be huge compared to the domain of interest. Even though an AMR feature is adopted, the total number of grid points can still be a big burden, slowing down the simulation.

The problem of a single bubble rising in a viscous liquid has been widely used as a typical validation case for the development of new numerical methods for multiphase flow [6, 40, 41]. Due to numerous experimental and numerical studies in the past, the physical understanding of the bubble rise behavior in liquid has been well-established in some flow regimes, e.g. regimes with lower Reynolds and Bond numbers [7, 1]. However, due to the complexity in multiphase flow physics and the difficulties in both experiments and simulations, the behavior of a rising bubble with high Reynolds number is not understood well [26, 21]. In this paper, we first validate our model through comparing computational results of a single bubble rising with experimental results [1] in aspects of both bubble shapes and terminal velocities. In addition, we apply the 3D model to simulate air bubbles rising in water, and we compare the terminal velocities of the bubbles predicted in our simulations with experimental results within a large range of diameters: from 0.5 mm to 30 mm. There have been few numerical studies on this except some recent ones [9, 21]. However, since air bubbles rising in water is such a common process both in our daily life and in industrial applications, a better understanding of this process is of great importance.

The rest of this paper is organized as follows. In Section 2 we present the governing equations as well as the numerical method we apply to solve these equations. Numerical results presented in Section 3 include a detailed sensitivity analysis of the computational set-up as well as validation through a comparison of our numerical predictions with available experimental data. Finally, we recapitulate our main findings in Section 4.

2. MATHEMATICAL MODEL AND NUMERICAL METHOD

2.1. Governing Equations

The problem of gas bubbles rising in liquids studied in this paper can be described as an isothermal, multi-fluid system with two incompressible and immiscible Newtonian fluids. We will use one single set of governing equations for the entire flow domain where we treat the different fluids as one single fluid with material properties varying across the interface. With this "one-fluid" approach, there is no need to deal with the jump conditions across the interface when the governing equations are solved. However, we will have to calculate the fluid property distributions and include the surface tension as a singular source term in the solution domain through the use of a delta function before the equations can be solved.

The mass conservation for the whole domain under the incompressibility condition may be expressed in form of volume flux conservation,

$$\nabla \cdot \mathbf{u} = 0 . \tag{1}$$

The momentum conservation (Navier-Stokes equations) takes the form,

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = -\nabla p + \nabla \cdot [\mu(\nabla \mathbf{u} + \nabla^{\mathrm{T}} \mathbf{u})] + \int_{\Gamma} \sigma \kappa \mathbf{n} \delta(\mathbf{x} - \mathbf{x}_f) ds + (\rho - \rho_l)\mathbf{g} , \tag{2}$$

where $\mathbf{u}$ is the fluid velocity, ρ is the fluid density, ρ_l is the density of the liquid phase, p is the pressure, μ is the fluid viscosity, σ is the surface tension coefficient, κ is the interface curvature, $\mathbf{n}$ is the unit normal vector to the interface, $\mathbf{g}$ is the gravitational acceleration, and $\delta(\mathbf{x} - \mathbf{x}_f)$ is a delta function that is defined as the product of three one-dimensional delta functions: $\delta(\mathbf{x}) = \delta(x)\delta(y)\delta(z)$, $\mathbf{x} = (x, y, z)$. The subscript f refers to a point on the interface Γ. It is worth pointing out that the material properties density ρ and viscosity μ will be discontinuous across the interface, and there will generally be a jump in the pressure p across the interface as well. Note that the surface tension term is a singular term that only comes into effect on the interface between the two fluids.

We non-dimensionalize the equations by introducing dimensionless characteristic variables as follows,

$$\mathbf{x}^* = \frac{\mathbf{x}}{D},\ \mathbf{u}^* = \frac{\mathbf{u}}{\sqrt{gD}},\ \tau^* = \sqrt{\frac{g}{D}}t,\ \rho^* = \frac{\rho}{\rho_l},\ p^* = \frac{p}{\rho_l gD},\ \mu^* = \frac{\mu}{\mu_l},\ \kappa^* = D\kappa,\ \mathbf{g}^* = \frac{\mathbf{g}}{g},$$

where D is the diameter of a sphere with the same volume as the bubble and $g = \|\mathbf{g}\|$. Thus we may re-express the Navier-Stokes equations as

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot\rho\mathbf{u}\mathbf{u} = -\nabla p + \frac{1}{Re^*}\nabla\cdot[\mu(\nabla\mathbf{u} + \nabla^{\mathrm{T}}\mathbf{u})] + \frac{1}{Bo^*}\int_\Gamma \kappa\mathbf{n}\delta(\mathbf{x} - \mathbf{x}_f)ds + (\rho - 1)\mathbf{g}, \quad (3)$$

in which the superscript * has been omitted for convenience. Note that the non-dimensional Reynolds and Bond numbers used here are thus defined as

$$Re^* = \frac{\rho_l g^{1/2} D^{3/2}}{\mu_l} \text{ and } Bo^* = \frac{\rho_l gD^2}{\sigma}.$$

By studying the non-dimensional formulation, it can be noticed that the flow is entirely characterized by the following four dimensionless parameters: The density and viscosity ratios of the fluids, the Reynolds number and the Bond number. It is also noted that the definition of the non-dimensional Reynolds number in the experimental works is different from the one defined here. Normally, experimental works prefer the following non-dimensional numbers: Eotvos number (E, also known as Bond number); Morton number (M) and Reynolds number (Re), defined as

$$E = \frac{\rho_l gD^2}{\sigma},\ \mathrm{M} = \frac{g\mu_l^{\,4}}{\rho_l\sigma^3},\ \text{and } \mathrm{Re} = \frac{\rho_l DU_\infty}{\mu_l},$$

where U_∞ is the terminal rise velocity of the bubble measured in the experiments.

2.2. Treatment of the Discontinuities across the Interface

When the governing Navier-Stokes equations are solved numerically on a fixed grid, the values of the density and viscosity on these grid points are required. It is a reasonable assumption that each fluid is incompressible, and fluid properties such as density and viscosity are constant in each fluid phase. Hence the density and viscosity are physically discontinuous across the interface between the two immiscible fluids, and this abrupt jump at grid points adjacent to the interface has traditionally caused great problems in

many numerical methods. In Tryggavson et al. [46, 45] a fixed background mesh is adopted to solve the governing flow equations, and a separated mesh is applied to track the position of the interface as well as the discontinuities across the front. An illustration of such a mesh system is shown in Figure 1. The discontinuities across the front are distributed from the front mesh to the background mesh, and continuous distributions of the fluid properties on the fixed background mesh can be reconstructed. The singular source term on the front is distributed to the background grid similarly, and the governing equations can thus be solved on the fixed background grid using any preferred numerical approach.

Let us first assume zero interface thickness. Consider the associated reconstruction of the field distribution $b(\mathbf{x},t)$ of material properties at time t in the whole domain through a certain indicator function $I(\mathbf{x},t)$. Let the indicator function be zero in the liquid phase and one in the gas phase. We may then write,

$$b(\mathbf{x},t) = b_l + (b_b - b_l)\cdot I(\mathbf{x},t), \tag{4}$$

where $b(\mathbf{x},t)$ is either fluid density or viscosity, and the subscripts l and b refer to liquid and gas phase, respectively. Further let Ω be the domain of the gas phase and let Γ be the interface between the two phases. The indicator function may then be expressed as

$$I(\mathbf{x},t) = \int_{\Omega(t)} \delta(\mathbf{x}-\mathbf{x}')d\mathbf{x}'. \tag{5}$$

Taking the gradient of the indicator function and applying Stokes' theorem, we get

$$\nabla I(\mathbf{x},t) = \int_{\Omega(t)} \nabla\delta(\mathbf{x}-\mathbf{x}')d\mathbf{x}' = \int_{\Gamma(t)} \mathbf{n}\delta(\mathbf{x}-\mathbf{x}')d\mathbf{s}, \tag{6}$$

where $\mathbf{n}$ is the outer unit normal vector of the interface. Taking the divergence yields a Poisson equation for the indicator function:

$$\nabla^2 I(\mathbf{x},t) = \nabla\cdot\int_{\Gamma(t)} \mathbf{n}\delta(\mathbf{x}-\mathbf{x}')d\mathbf{s}. \tag{7}$$

We solve this equation and then calculate the distribution of material properties from equation (4).

Unverdi and Tryggvason [46] addressed the sharp jump in fluid properties across the interface in their front tracking algorithm. They introduced an artificial thickness of the interface inside which the material properties vary continuously from one fluid to the

other. According to this idea, a distribution function $D(\mathbf{x})$ is introduced to approximate the delta function $\delta(\mathbf{x})$ with the assumption of an artificial thickness of the interface. We here adopt the traditional Peskin distribution function [31],

$$D(\mathbf{x}-\mathbf{x}_f)=\begin{cases}(4h)^{-3}\prod_{i=1}^{3}(1+\cos(\frac{\pi}{2h}|\mathbf{x}-\mathbf{x}_f|)) & \text{if } |\mathbf{x}-\mathbf{x}_f|<2h\\ 0 & \text{otherwise.}\end{cases} . \tag{8}$$

Substituting the Peskin distribution function into equation (7), the indicator function can be reconstructed by solving the Poisson equation. The resulting indicator function will then be zero in the pure liquid phase, vary continuously from zero to one in the artificial thickness region, and one in the gas phase.

Besides the discontinuity in fluid properties across the bubble interface, the surface tension, $F_\sigma=\int_\Gamma \sigma\kappa\mathbf{n}\delta(\mathbf{x}-\mathbf{x}_f)ds$, a singular source term on the bubble interface, brings another great challenge for numerical methods in multiphase flow. In the current study the net force caused by surface tension on the surface elements is calculated, thus circumventing the high-order derivatives involved in curvature calculations. Figure 2 shows the surface tension force exerted on a central surface element (E0) by its neighboring elements (E1, E2 and E3). The surface tension force acting on an edge shared between the central element and a neighboring element can be calculated by

$$\mathbf{F}_i=\sigma(\mathbf{t}_i\times\mathbf{n}_{i,0}) \quad \text{i}=1,2\text{ and }3\ , \tag{9}$$

where $\mathbf{t}_i$ is the vector of edge i and $\mathbf{n}_{i,0}$ its unit outer normal. Hence, for a central element E0, the net force caused by surface tension can be expressed as,

$$\mathbf{F}_{\sigma,E}=\sum_{i=1}^{3}\mathbf{F}_i=\sigma\sum_{i=1}^{3}(\mathbf{t}_i\times\mathbf{n}_{i,0})\ . \tag{10}$$

According to equation 10, the net surface tension force on all surface elements can be calculated and then distributed to the background mesh for solving the momentum equations:

$$\mathbf{F}_\sigma(\mathbf{x})=\sum_k\mathbf{F}_{\sigma,E}D(\mathbf{x}-X_k) \tag{11}$$

where X_k represents the mass centre of the k-th element used to triangulate the bubble surface.

2.3. Tracking the Moving Interface

With the techniques introduced in Sections 2.1 and 2.2, the governing equations can be solved on a fixed background grid to obtain the flow field. An adaptive, unstructured triangular mesh (front markers) is used to represent the interface between the two fluid phases. Hence, the velocity of the moving front markers can be obtained by interpolation from the flow field on the background mesh, and then the front mesh points can be advected in a Lagrangian manner. Thus the front moves with the same velocity as the surrounding fluid, and the so-called no-slip condition of the interface is satisfied. In this paper, the interpolation is carried out using the same distribution function as the one used for the transfer of fluid properties to the background grid:

$$\mathbf{u}_f(\mathbf{x}_f, t) = \sum_{\mathbf{x}} \mathbf{u}(\mathbf{x}, t) D(\mathbf{x} - \mathbf{x}_f), \tag{12}$$

$$\mathbf{x}_f^{\,n+1} = \mathbf{x}_f^{\,n} + \mathbf{u}_f^{\,n} \Delta t. \tag{13}$$

As the front marker points are advected, the mesh size and quality may consequently change. The resolution of the front mesh has a strong effect on the information exchange with the fixed background grid, which may eventually affect the accuracy of the simulation results. Therefore, it is of key importance that the front mesh has a more or less constant quality and uniform size throughout the duration of the simulation. To ensure this, the front quality is examined at each time step and adapted when necessary. In this paper, the resolution of the triangular mesh for the 3D surface of the bubble is maintained more or less uniform through adaptation as the interface evolves.

2.4. Mesh Adaptation

As two sets of mesh are applied in the current front tracking method, the resolution of the front mesh and the background mesh near the front plays an important role in resolving the interfacial physics of the multiphase flow. From physical principles it is known that fluid particles on the bubble interface will move downwards towards the bottom of the bubble as the bubble rises. Similarly, the mesh points also move downwards on the bubble surface in the front tracking method as the bubble rises. As a result, the mesh on the upper part of the bubble becomes coarser. On the other hand, the

mesh at the lower part of the bubble becomes increasingly dense. Figure 3(a) shows the variation of front mesh quality as the bubble rises in liquid without front mesh adaptation. It is obvious that the accuracy will be affected when the mesh on the top is too coarse, and that the dense fine mesh at the bottom of the bubble will consume excessive computing power without much benefit in accuracy. Thus, the front mesh adaptation as shown in Figure 3(b) is essential to ensure the accuracy and efficiency of the simulation.

In this aspect, three basic operations are adopted to adapt the front mesh, namely edge swap, edge split and edge deletion. For long edges, the edge swap operation as shown in Figure 4(a) is a simple and easy operation to improve the mesh quality. In the edge split operation as shown in Figure 4(b), a new point is generated by surface fitting of the existing neighboring mesh points. This new point is then inserted into the two associated meshes, and new and finer triangles are generated to replace the old ones. Thus edge split is important to refine the front mesh. For the deletion of short edges as shown in Figure 4(c), the triangles associated with the short edge will be deleted, and the resulted gap will be sealed through merging the old nodes of the short edge. Hence, edge deletion is important to coarsen the front mesh. In addition, consistent checking of the mesh connectivity is also important to ensure the accuracy in calculating the surface tension.

Accordingly, the resolution of the background mesh also plays an important role in capturing the flow behavior – particularly so in the vicinity of the interface. If the background mesh resolution is too low, then the detailed flow dynamics will not be captured reasonably well, resulting in unreliable and inaccurate simulations. Therefore, it is desirable to have relatively high-resolution grids, particularly near the interface, while coarse grids may be used away from the interface. This is achieved in our model by the use of the block-based adaptive mesh refinement (AMR) tool PARAMESH [24]. In this study, the refining and coarsening of the grid blocks is based on whether there exists a bubble front within the blocks. An example of the block-wise Cartesian mesh refinement generated by PARAMESH can be seen in Figure 5. It can be seen that fine background grids are located in the vicinity of the bubble, while coarser background grids are applied in regions further away from the bubble front. This feature makes it more efficient to solve the governing equations and to capture the flow physics near the interface accurately. An excellent feature of PARAMESH is that the Cartesian grid at all levels of

blocks has the same structure. Hence, once the flow solver is developed for one grid block, it can be easily applied to all levels of blocks. In addition, the different blocks can be distributed to different CPUs in an MPI parallel environment, which speed up the problem solving cycle.

2.5. Flow Solver

The numerical method for the governing flow equations is one of the key components in the simulation. Traditionally, an explicit projection-correction method based on second-order central differences on a regular, staggered Cartesian grid has been used along with the front tracking approach [46]. However, it seems that this approach is unable to handle the large density ratios typical of systems in industrial applications as well as in nature. In search of a more robust solver, Hua and Lou [17] implemented a modified version of the classical SIMPLE method [30] for axisymmetric multiphase flow. Further details about the modified SIMPLE algorithm can be found in the past works [17, 6]. Computational results indicate that this approach is more robust than the projection correction method – especially for multiphase flows with large density ratios such as the air-water system. This improvement is most probably due to the fact that the SIMPLE algorithm avoids solving the problematic pressure equation directly. Instead, the pressure and the velocity are corrected iteratively based on the governing equations.

2.6. Moving Reference Frame

In many applications of multiphase flow it is often desirable to study the long-term behavior and evolution of the moving interface between the fluids. In such applications the front may move a considerable distance, and the study of the rise path of an air bubble in water is a typical example. The computational domain must then be correspondingly large to accommodate such extensive movement. However, in a three-dimensional model with a high-resolution grid, a large computational domain is computationally very expensive. Computational cost may therefore limit the domain size and thus also long-time simulations.

To remedy this problem, we have therefore incorporated a moving reference frame into our numerical algorithm. The idea is to move the reference frame together with the

front such that the front (e.g. a bubble) remains more or less fixed in the computational domain. The size of the computational domain may then be chosen independently of the duration of the simulation, and this will in turn reduce the computational cost significantly. As a result, we may carry out long-time simulations of moving interface problems which could not be done in a stationary reference frame.

Figure 6 illustrates a moving reference frame. There, the frame XY stands for a stationary reference frame and the frame $X'Y'$ for a moving reference frame. The positions of a monitoring point in the frames XY and $X'Y'$ are represented as $\mathbf{x}_p$ and $\mathbf{x}'_p$, respectively, which are correlated with the position of the moving reference frame ($\mathbf{x}_m$) according to equation (14). The velocity of the monitoring point P is $\mathbf{u}(\mathbf{x},t)$ in the frame XY and $\mathbf{u}'(\mathbf{x}',t)$ in the moving frame $X'Y'$, and the velocity of the moving frame is $\mathbf{u}_m(t)$. The following correlation can be obtained:

$$\mathbf{x}_p = \mathbf{x}_m + \mathbf{x}'_p \tag{14}$$

$$\mathbf{u}(\mathbf{x},t) = \mathbf{u}_m(t) + \mathbf{u}'(\mathbf{x}',t)\,. \tag{15}$$

Allowing translational, but not rotational, movement of the frame in the present study, the following is the updated governing flow equations in the moving reference frame:

$$\begin{aligned}\frac{\partial(\rho\mathbf{u}')}{\partial t} + \nabla'\cdot\rho\mathbf{u}'\mathbf{u}' + \rho\frac{d\mathbf{u}_m}{dt} &= -\nabla' p + \frac{1}{Re^*}\nabla'\cdot[\mu(\nabla'\mathbf{u}' + \nabla'^{\mathrm{T}}\mathbf{u}')] \\ &+ \frac{1}{Bo^*}\int_\Gamma \kappa\mathbf{n}\delta(\mathbf{x}' - \mathbf{x}'_f)ds + (\rho - 1)\mathbf{g}\end{aligned}\,. \tag{16}$$

$$\nabla'\cdot\mathbf{u}' = 0 \tag{17}$$

The moving front will generally be accelerating and so will the moving reference frame. Thus the frame of reference in which we solve the governing equations is no longer an inertial frame, and we must therefore modify the momentum equations to take into account the acceleration of the frame. In addition, according to equation 15, when the governing equations are solved in a moving reference frame, the velocity condition on the boundary ($\mathbf{x}_B$') should be modified as $\mathbf{u}'(\mathbf{x}_B',t) = \mathbf{u}(\mathbf{x}_B,t) - \mathbf{u}_m(t)$.

Notice that the additional term on the left-hand side $d\mathbf{u}_m/dt$, which denotes the acceleration $\mathbf{a}_m$ of the moving reference frame, is added in Equation (16). We aim to choose $\mathbf{a}_m$ so that the rising bubble remains as fixed as possible in the moving frame, i.e. ideally the acceleration of the frame is equal to the acceleration of the bubble. The bubble acceleration is of course unknown, so we need to approximate this acceleration at each time step. We shall adopt the prediction as presented by Rusche [35], namely

$$\mathbf{a}_m^{n+1} = -\frac{\Delta \mathbf{u}_m^{n+1}}{\Delta t}, \tag{18}$$

where

$$\Delta \mathbf{u}_m^{n+1} = \lambda_1 \frac{\mathbf{x}_d^0 - \mathbf{x}_d^n}{\Delta t} - \lambda_2 \frac{\mathbf{x}_d^n - \mathbf{x}_d^{n-1}}{\Delta t}. \tag{19}$$

Here $\mathbf{x}_d^j$ is the position of the centre of mass of the bubble relative to the moving frame at time step j, $(\Delta t)^n = t^n - t^{n-1}$, and λ_1 and λ_2 are appropriate under-relaxation factors. It was found that $\lambda_1 = \lambda_2 = 0.1$ gave good results.

2.7. Solution Procedure

We may now summarize the main steps in advancing the solution from one time step to the next as follows:

(1) The velocity of the front marker points, $\mathbf{u}_f^n$, is calculated through interpolation of the fluid velocity field $\mathbf{u}^n$ according to Equation (12).

(2) The front is advected to its new position $\mathbf{x}_f^{n+1}$ by using the normal interface velocity $\mathbf{u}_f^n$ found in step (1) – see Equation (13). The front elements are then subject to examination for adaptation and topological change. Meanwhile, volume conservation is enforced.

(3) The indicator function $I^{n+1}(\mathbf{x}_f^{n+1})$ is computed based on the interface position $\mathbf{x}_f^{n+1}$. This is done by solving the Poisson problem in Equation (7) with the discrete delta distribution from Equation (8). Subsequently, the distribution of the

density ρ^{n+1}, the viscosity μ^{n+1} and the surface tension $\mathbf{F}_{\sigma}^{n+1}$ is updated on the flow solver grid points.

(4) We find the velocity field $\mathbf{u}^{n+1}$ and the pressure p^{n+1} by solving the mass continuity and momentum equations using a modified version of the SIMPLE algorithm. Appropriate boundary conditions are applied.

(5) Repeat steps (1) to (4) to advance the solution to time t^{n+2}.

3. RESULTS AND DISCUSSION

In this Section, we report various numerical results for different purpose, e.g. model sensitivity analysis, validation case, and model capabilities exploration. A summary of all the simulations cases can be found in Table I, in which all simulation parameters are listed.

3.1. Sensitivity Analysis - Size of the Computational Domain

Extensive experiments have been performed in the past to study the rise and deformation of single bubbles in quiescent liquids. Often these experiments have been done in large containers with a size of at least 20 bubble diameters in each spatial direction to avoid wall containment effects [1]. In this paper, we intend to validate simulation results against such experiments. To achieve this, the computational domain should also be rather large to avoid any significant effects caused by the wall confinement. On the other hand, if the domain is chosen too large, excessive computing time is needed to complete the simulation. To analyze the influence of the domain size, a number of numerical tests were run with domain sizes ranging from two to twelve bubble diameters in each of the spatial dimensions. The grid resolution was kept constant and accommodated approximately twenty cells inside the bubble in each direction. All computations were carried out in a moving reference frame.

The terminal rise velocity and the terminal bubble shape were used to assess the wall confinement effects for various domain sizes. The aim of this sensitivity analysis is to find the smallest possible computational domain in which wall containment effects have negligible impact on the bubble terminal velocity and shape. Figure 7 presents the

simulation results of the terminal bubble shape and the rise velocity using different domain sizes under the conditions of $\mathrm{Bo}^* = 243.0$, $\mathrm{Re}^* = 15.24$, $\rho_l / \rho_b = 1000$ and $\mu_l / \mu_b = 100$ (Case A3). There is a notable change in the terminal bubble shape and rise velocity as the domain size is increased from two to six bubble diameters. When the domain size is increased beyond six bubble diameters, no significant change in the simulation results is observed. Moreover, it is noted that the wall confinement has a strong effect on the terminal velocity for small domain sizes from two to six bubble diameters. However, the change in terminal velocity is only around 1% when increasing the computational domain size from eight to ten bubble diameters in each spatial dimension. Based on these observations we conclude that a domain size with side length of eight bubble diameters should be sufficient in our simulations. Actually, experimental results by Krishna et al. [23] also indicate that wall effects on a rising bubble is negligible when the diameter of the liquid container is larger than eight bubble diameters.

3.2. Sensitivity Analysis - Grid Resolution

PARAMESH divides the computational domain into a number of blocks in each spatial direction. Each block consists of a certain number of grid cells in each direction, and the governing equations are discretized and solved numerically on these grid cells. For a computational domain of fixed size, there are therefore two ways to change the grid resolution using PARAMESH: either by changing the number of blocks, which is determined by the maximum number of refinement levels, or by changing the number of cells in each block. In our grid sensitivity analysis we kept the maximum refinement level fixed and changed the number of cells in each block. All simulations were done in a moving, cubic computational domain with side length equal to eight bubble diameters using equal grid spacing in each of the spatial directions.

The results from the grid sensitivity analysis can be found in Figure 8 under the conditions of $\mathrm{Bo}^* = 243.0$, $\mathrm{Re}^* = 15.24$, $\rho_l / \rho_b = 1000$ and $\mu_l / \mu_b = 100$ (Case A3). It is noted that the terminal bubble velocity is highly sensitive to the mesh resolution up until 16 cells per bubble in each space direction. However, increasing the number of cells from 16 to 20 yields less than 1% change in terminal velocity. The terminal bubble shape also has a very strong dependence on the grid resolution - especially when the grid resolution

is relatively low. On the other hand, we can even see a slight change in shape when we increase the number of cells per bubble diameter from 16 to 20. However, increasing the number of cells per bubble diameter further to 32 does not lead to any visually detectable change in bubble shape. Based on the above we find it sufficient to use a resolution of 20 cells per bubble diameter in our simulations.

3.3. Comparison of Results Obtained in a Stationary and a Moving Reference Frame

Since a moving reference is introduced in this paper to perform long-time simulations of single bubbles rising as well as two-bubble interactions, it is important to evaluate the accuracy and impact of using a moving reference as opposed to a stationary frame. For this purpose, simulation results for Case A4 obtained in a stationary reference frame are compared with those obtained in a moving reference frame.

The bubble shapes predicted in both stationary and moving frames at different time steps are shown in Figure 9. There are no visually observable differences between the results from the two frames. A comparison of the velocity profiles of bubbles rising in a stationary and a moving reference frame is shown in Figure 10, and they are in reasonable agreement. Note that the velocity of the moving frame has been added to the rise velocity obtained in the moving reference frame to enable a direct comparison with the rise velocity in the stationary frame. In addition to comparing bulk behavior of rising bubbles, we would also like to compare the detailed flow patterns around the bubbles.

A comparison of the streamlines predicted in a stationary and a moving frame can be found in Figure 11. Since one frame is at rest and one is moving, comparing streamlines would only be sensible if we modify the velocity in one of the frames to account for the different velocities of the frames. Here we have chosen to subtract the velocity of the moving reference frame from the velocity field computed in the stationary frame before comparison. It can be seen from Figure 11 that an excellent agreement of the streamline patterns in the stationary and the moving frame is obtained. Furthermore, pressure distributions predicted in a stationary and a moving frame are compared in Figure 12, and again the results agree well.

Based on the various tests and comparisons of different flow characteristics carried out and described above, we can conclude that the use of a moving reference frame yields numerical results equivalent to those obtained in a stationary reference frame.

3.4. Model Validation with Experiments

In this section we will compare experimental results available in the literature [1] with predictions obtained by our numerical method. In Figure 13 we compare observed and predicted terminal bubble shapes for a range of Reynolds and Bond numbers, and the results agree very well. In Table II we compare the associated terminal rise velocities, and again there is reasonable agreement between experiments and our numerical predictions. However, note that the relative deviation in Case A1 is a little bit high. This may be due to the low rise velocity where the relative error will be high even though there is no change in the simulation accuracy.

Air bubbles rising in water are common in many industrial processes. Examples in chemical engineering include bubble columns, loop reactors, agitated stirred reactors, flotation, or fermentation reactors. For the design of efficient two-phase reactors, detailed knowledge of bubble sizes and shapes, slip velocities, internal circulations, swarm behaviors, bubble induced turbulence and mixing, and bubble size distributions (including coalescence and breakup) is of fundamental importance. In such industrial applications, bubbles often have non-spherical and even dynamic shapes as well as asymmetric wake structures. Extensive experimental studies have been performed to study air bubbles rising in water [7, 44]. Their measurements of the terminal rise velocity of air bubbles in water are presented in Figure 14 as a function of the bubble size. It is found that the measurements of the terminal velocity vary significantly (or bifurcation) when the bubble size is greater than 0.5 mm and smaller than 10 mm. Traditionally this variation has been explained by the presence of surfactants [7], but more recently both Wu and Gharib [47] and Tomiyama et al. [44] attributed this variation to the manner in which the initial bubbles were generated. The issue continues to be a matter of discussion - refer to Yang and Prosperetti [48].

Due to difficulties in measuring the physical properties on the bubble, a fundamental understanding of the system of a single bubble rising in high Reynolds number regimes is

not well-established. With the recent rapid increase in computing power, numerical simulations of two-phase flows based on continuum mechanics models with moving free interfaces have become feasible and proved extremely useful for a better understanding of fundamental processes and phenomena. However, numerical modeling of the multi-fluid system of air bubbles rising in water is still quite challenging due to the large density ratio of water to air, the low liquid viscosity of water, high Reynolds numbers, and large bubble deformations. Koebe et al. [21] started early trials of 3D direct numerical simulation of air bubbles rising in water at high Reynolds number using the volume of fluid (VOF) method. They studied bubbles with diameters from 0.5 mm to 15 mm, and their numerical predictions on the terminal rise velocity of the bubbles agree reasonably with experimental data. However, they introduced some initial white noise in the simulations, which may introduce non-physical perturbations to the simulation system. The recent work by Dijkhuizen et al. [9] reported their trial on simulation of single air bubbles rising in initially quiescent pure water using both a 3D front tracking method and a 2D VOF method for bubble diameters ranging from 1 mm to 8 mm. The calculated terminal rise velocites by the 3D front tracking method are quite close to the experimental observations by Tomiyama et al. [44], but they over-predicted the velocity for bubble diameters larger than 3 mm.

In this paper, we use the front tracking method with features of mesh adaptation and moving reference frame, allowing a finer mesh in the region of the bubble surface. Consequently, better accuracy is obtained in the current simulations. We simulate a single air bubble rising in initially quiescent pure water with the bubble diameters ranging from 0.5 mm to 30 mm. The numerically predicted rise velocities of the bubbles agree well with the upper bound of the experimental measurements by Tomiyama et al. [44] within the whole range of different bubble sizes. When the bubble diameter is in the range from 2.0 mm to 10 mm, oscillation of the bubble rise velocity and the bubble shape is also predicted in the simulations. The terminal bubble rise velocity is calculated through averaging the instantaneous rise velocity over a period of time. Since we assume the initial bubble shape to be spherical and the surface tension coefficient to be constant, the bifurcation of the bubble rise velocity is not revealed in the current simulation. However, this is an interesting topic to be explored in the future.

3.5 Numerical Studies on the Interaction between Two Rising Bubbles in Viscous Liquid

The problem of a single bubble rising in a viscous liquid is an ideal case for numerical model validation. However, the final goal when developing a numerical model for multiphase flow is not just investigating the flow behavior of single bubbles rising in viscous liquids, but also investigating multi-fluid systems with multiple bubbles. With the confidence from validating the current model for a single bubble rising in a viscous liquid, we would like to extend this model to explore the complex interaction between two bubbles rising in a liquid. Figures 15 and 17 illustrate the simulation of the interaction of two initially spherical bubbles rising in a quiescent liquid due to buoyancy.

In the first simulation, one smaller bubble is initially located 2.5D above a bigger bubble in vertical direction, and 0.5D axis-off from the bigger bubble in the horizontal direction of Y. Here, D represents the effective diameter of the bigger bubble. The diameter of the smaller bubble is half that of the bigger bubble. The flow conditions for the bigger bubble are as follows: $\mathrm{Re}^* = 134.6$, $\mathrm{Bo}^* = 115.0$ $\rho_l / \rho_b = 1181$ and $\mu_l / \mu_b = 5000$ (Case B1). Figure 15 shows the temporal bubble shape evolution of two rising bubbles. As the bigger bubble has a higher rise velocity, it will catch up with the smaller bubble (Figure 15($\tau = 4.0$)). When they are close enough, the trailing bigger bubble is significantly affected by the low-pressure zone in the wake of the leading smaller bubble. The trailing bubble undergoes large deformations and moves towards the bottom wake zone of the leading bubble (Figure 15($\tau = 6.0$)). Finally, the trailing big bubble merges with the leading smaller bubble, and a toroidal bubble ring is formed (Figure 15($\tau = 10.0$)). Similar bubble shape evolution patterns have also been predicted by other numerical predictions [40]. In addition, Figure 16 shows the temporal variation of the position of the bubbles in both vertical and horizontal directions. It can be seen from Figure 16(a) that the trailing bigger bubble has a higher rise speed than the smaller leading bubble. The interesting finding is that when the two bubbles are close enough, then the rise speed of both bubbles increases significantly. After the coalescence of the two bubbles, the resulting merged bubble returns to a normal situation of a single bubble. The lateral movement of the trailing bubble caused by the leading bubble can be seen in Figure 16(b). Even though initially the leading bubble moves slightly away from the trailing

bubble laterally, this distance is quite small. However, the trailing bubble, despite its big size, is significantly affected by the leading bubble and moves towards it.

In the second simulation, the smaller bubble is initially located 2.5D above the bigger bubble in vertical direction, and 1.0D center-off from the big bubble in the horizontal direction of Y. Here, D represents the effective diameter of the bigger bubble. The diameter of the smaller bubble is half that of the bigger bubble. The flow conditions for the bigger bubble are as follows: $\mathrm{Re}^* = 15.24$, $\mathrm{Bo}^* = 243.0$, $\rho_l / \rho_b = 1181$ and $\mu_l / \mu_b = 5000$ (Case B2). Figure 17 shows the temporal evolution of the two rising bubbles. As a result, in this case the bigger bubble finally overtakes the smaller one, since the big bubble is further horizontally off-set the small one. It can be seen from Figures 17 and 18(b) that the leading bubble first starts moving laterally away from the trailing bubble, whereas the trailing bubble then starts moving towards the leading bubble before the overtaking occurs (Figure 17($\tau = 4.0, \tau = 6.0, \tau = 8.0$)) . After the bigger bubble has overtaken the smaller one, the smaller bubble is significantly affected by the wake of the bigger bubble. In fact, the smaller bubble is attracted to the wake of the bigger bubble, resulting in a highly deformed and elongated bubble shape as shown in Figure 17 ($\tau = 12.0, \tau = 14.0, \tau = 16.0$). It is also noticed from Figure 18(a) that the smaller bubble is accelerated and rises fast in the wake of the bigger bubble, and finally it catches up and merges with the bigger bubble (Figure 17($\tau = 18.0, \tau = 20.0, \tau = 22.0$)). In this case, the smaller trailing bubble has little effect on the rising speed of the bigger leading bubble.

4. CONCLUSION

The numerical algorithm used in this paper is a further extension of the algorithm given in [17] for simulating 3D gas bubbles rising in viscous liquids at high Reynolds and Bond numbers for systems with large density and viscosity ratios such as air/water. To achieve this, mesh adaptation is implemented for both the front mesh and the background mesh, and a moving reference frame attached to the rising bubble is used to solve the governing incompressible Navier-Stokes equations. The solution method is a finite volume scheme based on the Semi-Implicit Method for Pressure-Linked Equations

(SIMPLE), and the solver appears to be robust even in the range of high Reynolds numbers and high density/viscosity ratios. The bubble surface is tracked explicitly using an adaptive, unstructured triangular mesh. The model is integrated with the software package PARAMESH, a block-based adaptive mesh refinement (AMR) tool developed for parallel computing. It includes features such as background mesh adaptation and parallel implementation of solvers for the governing equations on supercomputers. The interpolations between the front mesh and the background mesh are done with Peskin's traditional approximation of the delta function. The current model has been applied to simulate a number of examples of 3D gas bubbles rising in viscous liquids, e.g. air bubbles rising in water. The simulation results are compared with experimental observations in aspect of both the terminal bubble shape and the terminal bubble velocity. In addition, we use this model to simulate the interaction between two bubbles rising in liquid. The simulation results provide us with some physical insights into the complex behavior of bubbles rising in viscous liquids.

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